

Isobutyric anhydride
97-72-3 | DTXSID7026609

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.64

Global applicability domain: Inside

Local applicability domain index: 6.06e-01

Confidence level: 7.32e-01

Nearest Neighbors from the Training Set

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tert-Butyl acetate

Measured: 1.76

Predicted: 1.61

Image not found

tert-Butyl methacrylate

Measured: 2.54

Predicted: 2.28

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5,5-Dimethylhexane-2,4-dione

Measured: 1.67

Predicted: 1.83

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4-Methyl-2-pentanone

Measured: 1.31

Predicted: 1.43